

## Microstructure of Complex Fluids Including Surfactants, Copolymers, and Tethered Copolymers from Density Functional Theory

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In many applications involving complex fluids, the local microstructure or heterogeneity determines the properties of the macromolecular system. Such applications of macromolecular fluids are wide ranging and include performance polymers, synthesis of nanomaterials, copolymer films and coatings, and chemically modified surfaces for sensors. To design and control such systems with confidence, a successful model must incorporate molecular features on a range of length scales while remaining computationally tractable. What has been lacking is a theory that incorporates molecular features in multicomponent mixtures including explicit solvent, polymers and nanoparticles, uses potential models transferable with molecular simulation that include directional interactions like hydrogen bonding, and naturally models even trace components. We believe that classical density functional such as iSAFT based on Wertheim's theory for associating molecules fills this void. Recent extensions of iSAFT to predict the effects of hydrogen bonding and bond flexibility in polymer systems are presented. Applications of the theory demonstrate methods to control microstructure of surfactants, block copolymers, and grafted polymers as stimuli responsive materials.